Oklahoma NSF EPSCoR Research Connection

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Inside this issue:

Oklahoma Receives $15 Million Award to Boost Biofuels Research

Submitted by: Ms. Shelley D. Wear, Special Programs Coordinator, Oklahoma EPSCoR

At a time when Americans are dealing with fluctuating fuel costs, Oklahoma's scientists are stepping up the pace on research to develop efficient alternative fuels from switchgrass and other non-food crops.

To aid with the state's research in bioenergy, Oklahoma has been awarded $15 million over five years from the National Science Foundation (NSF) Experimental Program to Stimulate Competitive Research (EPSCoR). The Oklahoma State Regents for Higher Education will provide an annual $1.1 million match. The award will contribute to Oklahoma's leadership in the national effort to gain energy independence by utilizing biofuels.

The NSF award is a multi-institutional collaborative project that includes researchers from Oklahoma State University, the University of Oklahoma and the Samuel Roberts Noble Foundation. The award will be managed by Dr. James Wicksted, principal investigator and OSU physics department chair, and Dr. Frank Waxman, co-principal investigator and Oklahoma EPSCoR state director. Dr. Raymond L. Huhnke, OSU professor of biosystems and agricultural engineering, will serve as the team's lead researcher working with 12 other scientists on the project.

Building on Oklahoma's strengths in genomics research, scientists will develop methods to increase biomass yield to produce ethanol from non-food crop sources such as switchgrass. The project will also focus on enhancing biofuel refining using fermentation by microorganisms and chemical catalysis.

> ***Oklahoma's scientists are stepping up the pace on research to develop efficient alternative fuels from switchgrass and other non-food crops.***

"I am extremely proud that our Oklahoma research universities have been so successful when competing for EPSCoR grants. The success of the Oklahoma EPSCoR and DEPSCoR programs is a testament to the talented professors and students that are attracted to our highly esteemed universities. I congratulate the Oklahoma EPSCoR program for receiving this award, which will further our nation's quest to achieve greater energy security," said Sen. Jim Inhofe, who has been a steadfast supporter of federal EPSCoR programs.

The award will offer research opportu-

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EPSCoR Director Inducted into Hall of Fame

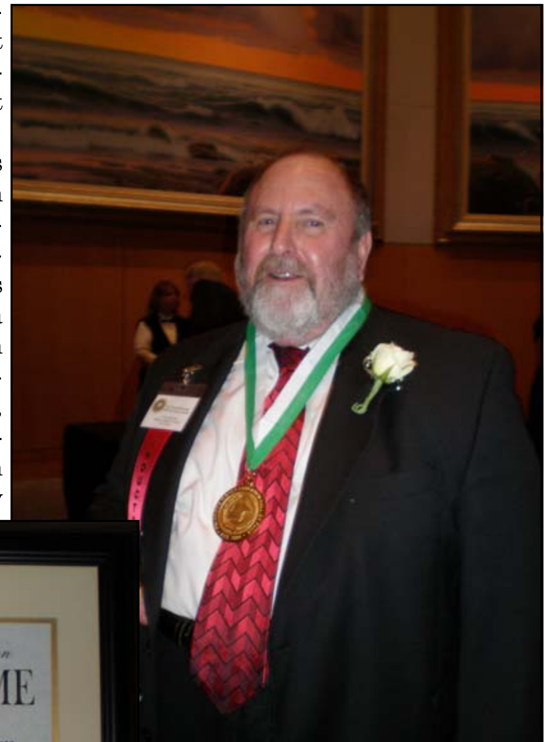
Submitted by: Shelley D. Wear, Special Programs Coordinator, Oklahoma EPSCoR

State EPSCoR Director and Professor of Microbiology and Immunology at the University of Oklahoma Health Science Center (OUHSC), Dr. Frank Waxman, was recently inducted into the Oklahoma Higher Education Hall of Fame. Waxman was one of ten distinguished individuals receiving this honor at the National Cowboy and Western Heritage Museum in Oklahoma City on Tuesday, October 7, 2008. His induction reflects his outstanding contributions to higher education, research and economic development in Oklahoma.

Student education and faculty research at community colleges, regional universities, and research campuses across the state have been positively influenced by Waxman's visionary leadership. During his career, Waxman successfully obtained and administered more than $50 million in research grants, a prodigious contribution to Oklahoma's competitiveness for research and development (R&D) funding. His leadership in curriculum reform and research, combined with a strong commitment to increase opportunities for underrepresented minorities, have resulted in strong partnerships and collaborations between students, faculty and administrators and among higher education and research institutions statewide.

Waxman's own research has served as a bench-mark study in the discipline of immunology and is widely published in medical textbooks. He was a co-founder of a biotech company that was listed on the NASDAQ and served as vice president for research (VPR) at OUHSC, where his leadership was instrumental in establishing policies and procedures for developing intellectual property. During his tenure as VPR, Waxman encouraged faculty to pursue patent protection for emerging technologies, facilitated the grant application process and improved surveillance on grant compliance.

Waxman currently serves as principal investigator (PI) on two of Oklahoma's largest research grants aimed at increasing the state's competitiveness for R&D funding. As PI on a National Science Foundation EPSCoR Research Infrastructure Improvement (RII) grant, he leads efforts to propel Oklahoma to national prominence in the areas of nanotechnology and plant virus biodiversity and ecology. As PI on the Oklahoma Biomedical Research Excellence (INBRE) grant, funded by the National Institutes of Health, he leads efforts to develop a more interdisciplinary undergraduate curriculum, build infrastructure in targeted areas and to recruit and retain excellent biomedical scientists in Oklahoma. Both grants promote interdisciplinary research, provide for infrastructure improvement and build human resources in the sciences with numerous opportunities for graduate and undergraduate students and faculty.



The Hall of Fame was established in 1994 by the Oklahoma Higher Education Heritage Society to recognize outstanding women and men who have excelled in higher education and who have encouraged others to contribute to the economic development and quality of life in Oklahoma. One hundred and fifty-six leaders have been inducted into the Hall of Fame since conception.

The EPSCoR staff express our congratulations to Dr. Waxman for achieving this high honor marking his leadership and excellence in education and research that has helped to increase opportunities for Oklahoma students on all levels to experience the excitement of science.

Award history and Waxman's biosketch courtesy of the Oklahoma Higher Education Heritage Foundation www.ohehs.org . Photos by Jennifer Hamm.

Solving Bigger Challenges: Modern Applications of Molecular Thermodynamics

Submitted by: Dr. Alberto Striolo, Assistant Professor, School of Chemical, Biological and Materials Engineering, University of Oklahoma

The name '*thermodynamics*' derives from the Greek '*therme*', heat, and '*dynamics*', power. In the 18-19th century the success of this discipline produced the steam engine. Since then, thermodynamics experienced several 'adaptations', one of which occurred in 1969, with the publication of the book '*Molecular Thermodynamics of Fluid-Phase Equilibria*'. The author, John M. Prausnitz, is widely recognized as '*the father of modern chemical engineering thermodynamics*' because he refocused the modern applied thermodynamics research on understanding the properties of molecules, and on how to relate such properties to macroscopic quantities such as pressure and temperature. Within this vision, our group at OU believes that modern thermodynamics, which we like to term '*molecular science and engineering*', could help us solve some of the great contemporary challenges. These include, but are not limited to finding alternative energy sources, fighting debilitating diseases, providing potable water, and preserving our environment.

In support of my argument, I present below three examples from the research conducted within my group at OU. The interested reader is referred to our website for further information: http://hotohke.ou.edu/~astriolo/.

The first example focuses on the transformation of raw agricultural products to biofuels. Such processes often rely on metal particles, the catalysts, to speed up chemical reactions. Our group is interested in understanding how a small cluster of, *e.g.*, 13 platinum atoms (Pt13) can promote one desired chemical reaction. To tackle this problem we study the distribution of electrons around the metal particle using *ab initio* density functional theory (DFT) methods. In **Fig. 1** we report the highest occupied molecular orbital, HOMO, for one platinum cluster atoms isolated (left), or in contact with one ***C* = *O*** molecule (right). The interesting result, in our opinion, is that as ***C* = *O*** approaches, the electronic distribution (HOMO) changes quite dramatically. We believe that this electronic structure change is responsible for speeding up chemical reactions, and we expect that clusters of various sizes and shapes will have different electronic structures. Our research will identify the best cluster to produce biofuels.

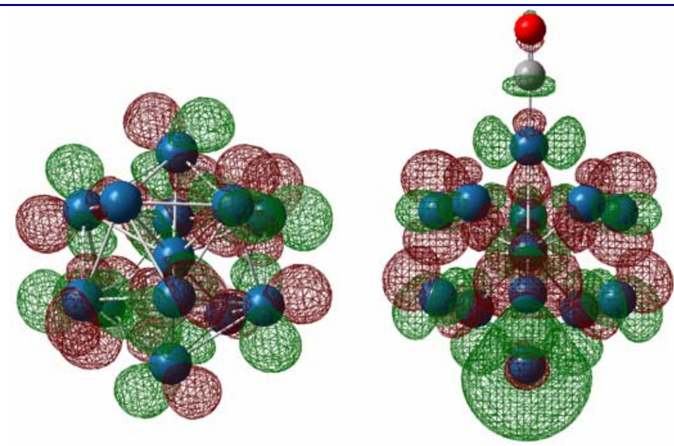


Fig. 1. Highest occupied molecular orbitals for bare Pt13 (left) and Pt13 with an adsorbed CO molecule (right). Platinum atoms are blue, carbon atoms are gray, and oxygen atoms are red. The data indicate how the electronic structure of the platinum cluster changes as the C = O molecule approaches it. These calculations provide us with vibration frequency for the absorbed C = O molecule, to be compared to experimental data.

As second example I would like to mention our studies on water, and aqueous electrolyte solutions, near solid surfaces. In **Fig. 2** we report the planar density profiles observed for water molecules near a fully hydroxylated silicon dioxide surface (*i.e.*, a grain of sand). These results are obtained conducting molecular dynamics simulations in which we describe the forces

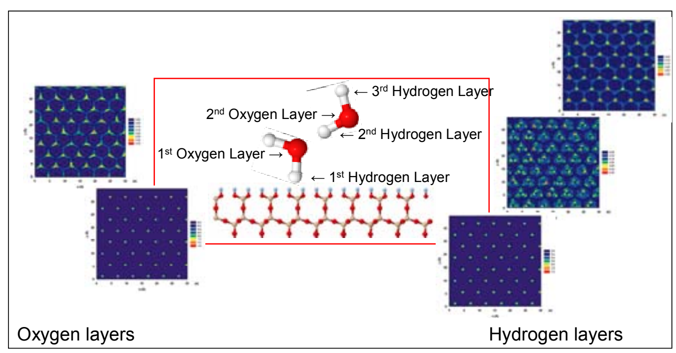


Fig. 2. Equilibrium molecular dynamics simulation results obtained for a thin water film deposited on a fully hydroxylated silicon dioxide surface. The surface is represented at the center (red, yellow, and light blue spheres are oxygen, silicon, and hydrogen atoms, respectively). The results are shown in terms of the density of O (left panels) and H atoms (right panels) belonging to water molecules on planes parallel to the surface but at various distances from it. The brighter the color, the higher is the probability of finding the atoms in the various locations. The results indicate that the surface yields an ordered structure for interfacial water that extends a few molecular diameters into the liquid phase.

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Switchgrass Research Studies Symbiosis Critical to Increased Biomass Production

Submitted by: Dr. Kelly D. Craven, Assistant Professor, Plant Biology Division, Samuel Roberts Noble Foundation

Switchgrass (*Panicum virgatum* L.) is a perennial C_4 grass native to North America, primarily in the tall-grass prairie regions of the Great Plains. The U.S. Department of Energy (DOE) has identified switchgrass as a promising bio-energy crop for cellulosic ethanol production because of its abundant biomass, excellent nutrient-use efficiency, and broad adaptability. Switchgrass has tremendous potential to serve both as an alternative to corn for ethanol production and as a valuable tool in ecological and environmental restoration efforts. The DOE has set a goal to replace 30% of current U.S. petroleum consumption with bio-ethanol by 2030. This will require billions of tons of biomass annually, with the contribution of perennial crops predicted to account for approximately 342 million tons. If switchgrass is to be a central component of this strategy, perhaps contributing up to 70% of this amount, approximately 15 million hectares need to be dedicated to switchgrass at a productivity level of 16 Mg ha^{-1}. The acreage dedicated to switchgrass would increase dramatically if the estimates are based on biomass yields (5.2 to 11.1 Mg ha^{-1}) obtained from recent on-farm experiments in marginal lands. Therefore increasing switchgrass productivity is paramount to implementing a sustainable approach to meet the demand for cellulosic biomass.

The profitability of switchgrass as a forage or biomass crop can be enhanced if yield can be increased with a concomitant decrease in chemical inputs, particularly N and P fertilizers. One means of accomplishing this is through utilization of symbiotic relationships wherein a microbial partner provides or enhances nutrient acquisition for its plant host. Dr. Kelly D. Craven, Assistant Professor, Plant Biology Division, Samuel Roberts Noble Foundation (SRNF) and his research group studied the stability of artificial associations between switchgrass and the ectomycorrhizal fungus, *Sebacina vermifera*, and potential benefits of this association in seed germination and biomass production. Culture filtrates from some strains of *S. vermifera* increased seed germination in the switchgrass cultivar Kanlow by 52%. Those strains had a high frequency of colonization on roots of selected populations of genotype Alamo even after two months of inoculation (Fig. 1). The positive effects of the association were reflected in biomass production and biomass related parameters. Inoculated plants were significantly taller, and produced as much as 113% more dry biomass than uninoculated control plants (Fig.2). This study illustrates the great potential of this association to increase biomass production and productivity of switchgrass. Long term benefits of the association in switchgrass are being investigated.

Dr. Craven was hired at SRNF as a result of the NSF RII grant EPS-0447262 in efforts to increase the critical mass of researchers working in the plant virus biodiversity and ecology field of study.

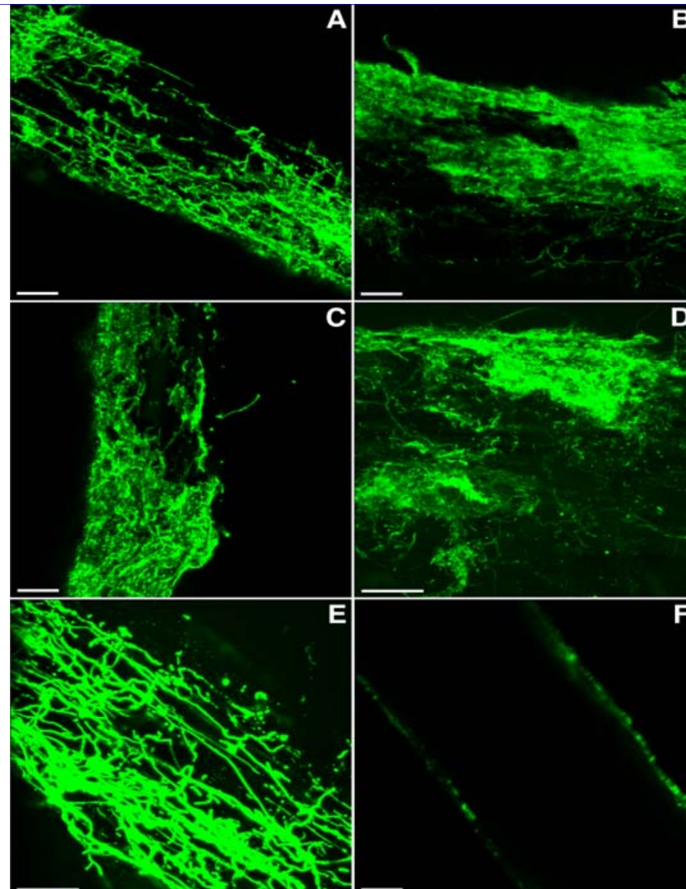

Fig. 1 Colonization of switchgrass and barley roots by *S. vermifera*. Switchgrass root colonization by strains MAFF-305828, MAFF-305830, MAFF-305835 and MAFF-305838 (A-D, respectively); MAFF-305830 colonized barley root (E) and uninoculated control switchgrass root (F). Root staining was performed using WGA-AF 488 and scale bar is 50 µm.

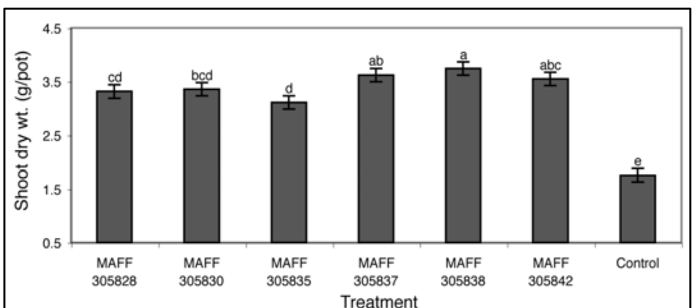

Fig. 2 Effect of *S. vermifera* strains on the shoot dry weight of switchgrass. Error bars are LSD, and the bars labeled with different letters are statistically significant (p< 0.05).

Acknowledgements: Supporting statistical information provided by the Department of Energy and The Bioenergy Science Center.

OK Research Infrastructure Improvement Award Biofuels Research Team Leaders

Oklahoma State University

- **Raymond L. Huhnke,** Department of Biosystems & Agricultural Engineering
- **Ramamurthy Mahalingam and Ramanjulu Sunkar**, Department of Biochemistry and Molecular Biology
- **Yanqi Wu**, Department of Plant and Soil Sciences

University of Oklahoma

- **Lance Lobban**, **Richard Mallinson, Daniel Resasco**, and **Alberto Striolo**, School of Chemical, Biological and Materials Engineering
- **Ralph Tanner**; Department of Botany and Microbiology
- **Zhili He** and **Jizhong Zhou**, Institute for Environmental Genomics

Samuel Roberts Noble Foundation

- **Kiran Mysore,** Plant Biology Division
- **Zengyu Wang**, Forage Improvement Division

$15 Million Award *(continued from page 1)*

nities for college faculty, undergraduate and graduate students, in addition to educational outreach initiatives aimed at K-12 public schools. Events such as Research Day at the Capitol, women in science conferences and grantwriting workshops will also receive support. The project will integrate research and education and foster a new cyberinfrastructure initiative.

"This award will strengthen Oklahoma's research capacity through a variety of educational initiatives designed to broaden participation in the science, technology, engineering and mathematics fields," said Chancellor Glen D. Johnson. "As a result, Oklahoma will have a stronger, more diverse scientific workforce prepared to invent and utilize new technologies needed to solve critical problems we face today, such as the need for alternative fuel sources."

"The NSF EPSCoR award is a vote of confidence for the state and will contribute toward ongoing efforts by Oklahoma's scientists to take the lead in bioenergy research. Oklahoma is committed to the development of viable alternative fuels and other forms of bioenergy that will aid in reduction of national dependence on foreign oil sources to meet the U.S. energy demands," said Oklahoma Secretary of Energy David Fleischaker.

The scientific leadership for the new NSF award will work closely with Fleischaker and the Oklahoma Department of Energy to advance the state's bioenergy industry in hopes of easing the uncertainty in fuel costs in the near future.

EPSCoR, originally developed by the NSF 28 years ago, is designed to expand research opportunities in states that have traditionally received less funding in federal support for university research. Oklahoma EPSCoR is a partnership among colleges and universities, industry, and research institutions. Its mission is to make Oklahoma researchers more successful in competing for research funding. Specific goals, objectives and strategies are developed for each federal EPSCoR program, based on federal and state needs.

Global Center for Viruses in Ecology Proposed to NSF

Submitted by: The Plant Virus Ecology Network

The environmental issues humanity currently faces are numerous and complex. Many share a need for science-based assessments of likely ecological outcomes resulting from scenarios of societal action. Microbial dynamics is central to predictions about ecosystem response to perturbation. Among microbes, least understood are viruses. Undeniable is that viruses are widespread, that they operate in intimate association with hosts, and that they have tremendous potential to cause epidemics, decimating hosts. Organisms with pathogenic capacity, such as viruses, are among those most likely to respond to perturbations in unpredicted, yet serious, ways and are also among those which may be manipulated by humans with nefarious intent. The need to understand virus ecology and evolution better is evident and recognized worldwide. However, this area of inquiry represents one of the last frontiers, in which much remains truly unknown.

To develop critical, cornerstone information about viruses for global environmental science, a team arising from the Plant Virus Biodiversity and Ecology (PVBE) scientific theme area of the now concluding round of NSF EPSCoR support proposed a “Center for Viruses in Ecology”, which would provide essential stimulus and momentum to the effort to describe plant virus distributions. It would develop mechanistic understanding of their roles in nature and their responses to human-mediated perturbations. The team is asking NSF to consider funding such a Center at a level of $5 million per year for five years. The Center would involve scientists from four Oklahoma institutions, nine institutions across the country and several institutions around the world.

The Center would focus on the ecological roles of plant-associated viruses in managed and unmanaged ecosystems (and exchanges between these systems), and would investigate the reciprocal influence of ecosystem properties on the distribution and evolution of plant viruses. The Center will undertake nationwide sampling of plants from natural and agricultural environments for identification of viruses and will conduct laboratory and field experiments testing hypotheses on the ecological relationships of plants, vectors and viruses. The Center will engage school children from various parts of the US in the collection of samples from plants, plant mixtures, arthropods, and water.

Logo of the Plant Virus Ecology Network, an NSF-funded Research Coordination Network that arose from the PVBE project and laid the groundwork for a Center funding application.

SOLVING BIGGER CHALLENGES

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acting between each water molecule and the solid surface. The results show a well-defined structure for interfacial water at room conditions. We are now exploring whether salts like NaCl (*i.e.*, the cooking salt) accumulate near the surface rather than keeping away from it. Designing surfaces that accumulate salts on them will allow us to purify saline water for human consumption.

I chose the third example from the area of materials design. Our group is interested in improving the intrinsic properties of fluids, such as hydrofluorocarbons, commonly used in refrigeration and air conditioning. Both technologies have tremendously improved life, especially in the Southern States, but require large amounts of energy. Typically, heat is transferred from a region at low temperature to the external environment, at higher temperature, using working fluids with large heat capacity and heat-transfer properties. To reduce the high energy requirements, we aim at improving the heat-transfer properties of the working fluids. One possible solution is to incorporate small components (*e.g.*, one-atom-thick layers of carbon atoms, known as graphene sheets) with large heat-transfer properties within the working fluid. To employ the graphene sheets we first require preventing their agglomeration during operation. Our recent results, obtained by conducting molecular dynamics simulations, suggest that functionalizing the carbon atoms at the edge of the graphene sheets is a viable strategy for these purposes.

We hope this brief review has convinced the reader that mastering the original thermodynamics principles will allow us to overcome many modern challenges, both those that we encounter today, and likely those that will present in the years to come.

We benefit tremendously from the effort of the OK EPSCoR administrators to stimulate collective scientific efforts, the *conditio sine qua non* for the success of any modern research enterprise. Because of space limitations, I cannot thank here all the people and institutions who are supporting our work. However, I must thank my research group members, who conduct all the work presented here, and more. These are Naga Rajesh Tummala and Brian Morrow, who initiated the group in 2005, Dimitrios Argyris, who joined in 2006, Deepthi Konatham and Shi Liu, who have been with us since 2007.

Upcoming Events 2008-2009

2008 Events

November 14 — **Oklahoma Research Day,** Northeastern State University, Broken Arrow Campus, OK

2009 Events

February 3 — **Women in Science Conference 2009**, Science Museum Oklahoma, Oklahoma City, OK

April 16-18 — **National Conference on Undergraduate Research (NCUR) 2009**, University of Wisconsin, La Crosse, WI

April 16-19 — **American Indian Symposium**, Northeastern State University, Tahlequah, OK

OTHER UPCOMING EVENTS

- **Annual State Conference 2009**
- **Donald W. Reynolds Oklahoma Governor's Cup 2009**
- **NSF Grants Workshop 2009**
- **Research Day at the State Capitol 2009**

For more information, please visit our website or contact Ms. Shelley D. Wear, Oklahoma EPSCoR Special Programs Coordinator at 405.225.9287 or swear@osrhe.edu.

www.okepscor.org/events.asp

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